Polar-Induced Electrostatic Control of Magnetism in Multiferroics/Insulator Heterostructure: T-$BiFeO_3$/$LaAlO_3$ system

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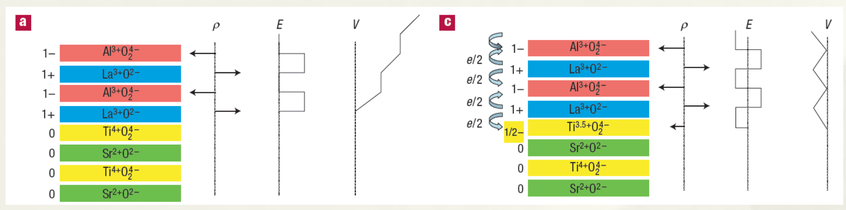
We predict a strong electrostatic control of magnetic coupling in the heterostructure system with two insulating transition-metal oxides, of which one is multiferroics. By employing first principle calculation, we consider an example of the tetragonal-like $BiFeO_3$/$LaAlO_3$ (T-BFO/LAO) system to illustrate the magnetoelectric coupling of the first $BiFeO_3$ layer at interface. The total energy calculation with different magnetic states shows the different magnetic coupling with distinct interface terminal type and ferroelectric polarization. The study on the electronic structure shows gapless interface states and indicates an electronic reconstruction emerging at the each polarized interface, leading to the metallic $Fe^{(3-\delta)+}$ and $Fe^{(3+\delta)+}$ oxidation state respectively, which eventually exhibits different magnetic behaviors.

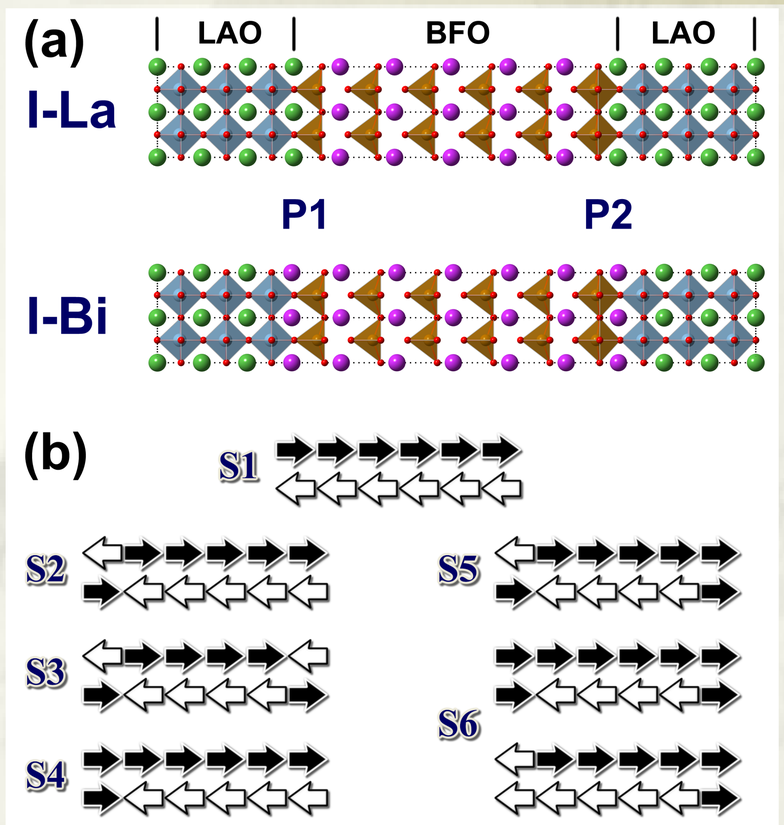
Intro. : Polar Catastrophe



The polar catastrophe illustrated for atomically abrupt (001) interfaces between $LaAlO_3$ and $SrTiO_3$

From: N. Nakagawa, H. Y. Hwang, and D. A. Muller, Nat. Mater. **5**, 204 (2006)

Structure & Spin Order: T-BFO/LAO



(a) Simulation models of T-BFO/LAO slabs with two structures, I-La and I-Bi. The green, violet and red balls correspond to La, Bi and O atoms, respectively. The brown and blue gray polyhedra are FeO_6 and AlO_6 octahedra. **(b)** Side view of six magnetic states S1-S6 using for calculation for both I-La and I-Bi. Both two configurations in S6 have been considered and are identical in energy.

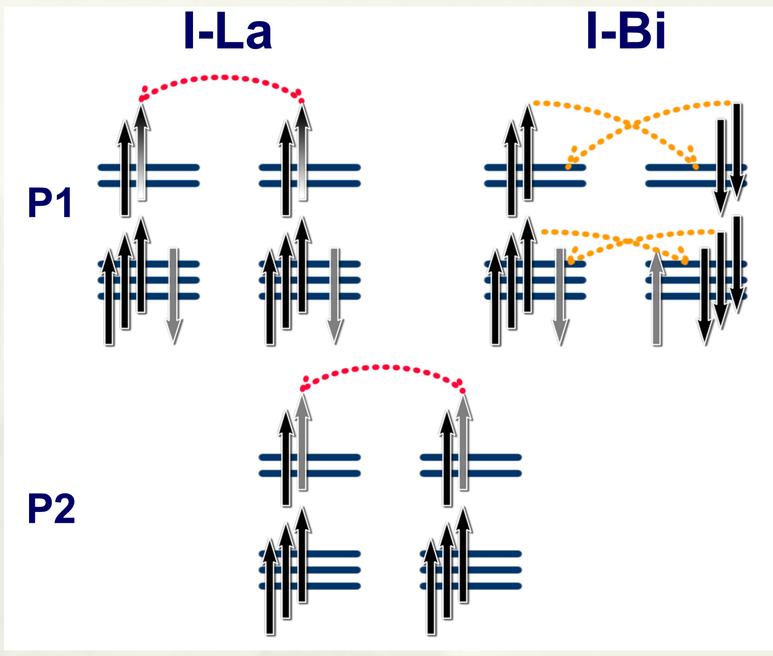
strong magnetoelectric coupling

Calculated in-plane and out-of-plane nearest-neighbor coupling parameters, J_{xy} and J_z, for bulk T-BFO and interfaces P1 and P2 in both I-La and I-Bi. Positive/negative values correspond to AFM/FM coupling, respectively. The local magnetic moments of Fe atoms have been normalized to $S = 1$.

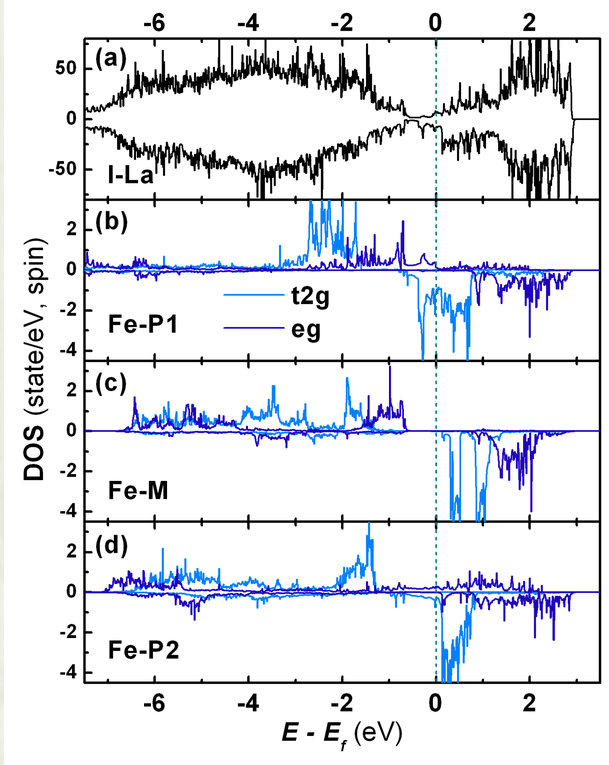
(meV)	Bulk T-BFO	I-La		I-Bi	
		P1	P2	P1	P2
J_{xy}	65.3	-11.5	-30.7	60.5	-28.6
J_z	-6.55	31.0	-3.7	7.5	-2.5

P1: $Fe^{(3-\delta)+}$ ($3d^{5+\delta}$)
I-La: FM
I-Bi: AF

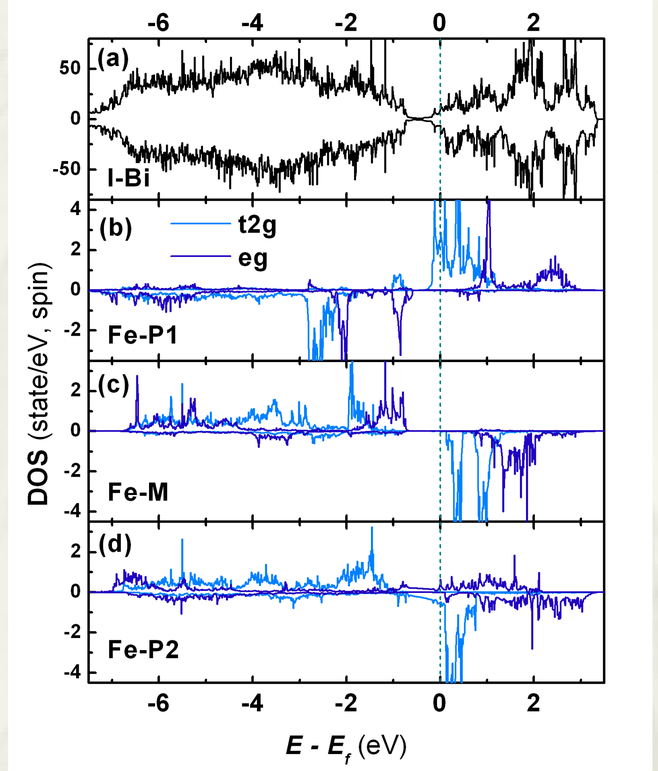
P2: $Fe^{(3+\delta)+}$ ($3d^{5-\delta}$)
I-La: FM
I-Bi: FM



DOS:I-La



DOS:I-Bi



In structure I-La,(left)/I-Bi(right) **(a)** the total density of state (DOS) and orbital-resolved projected DOS (PDOS) for Fe atoms at the fourth FeO_2 layer from P1 **(c)**, and at the interface P1 **(b)** and P2 **(d)**. Positive/negative values correspond to the spin up/down channel. The t_{2g} and e_g characters are shown in different color. The Fermi energy is set at zero

Why are magnetic couplings different in I-La and I-Bi at interface P1?

The volume of octahedral BO_6 (B = Fe, Al) with various positions under **(a)** state S1 and **(b)** each ground magnetic state, S6 and S5, respectively, in both I-La and I-Bi structures. **(c)** Schematic diagram of Fe atoms at P1 and P2, where brown, green and violet balls correspond to Fe, La and Bi atoms, respectively. This shows that the absence of lone-pair 6s electrons (the oval with $2e^-$) only affects ligand field of Fe at P1.